

Development of a General Reporting Program for Measurement Uncertainty

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Abstract—a computer program, named Uncertainty-Bot, has been developed for calculating and reporting measurement uncertainty. In order to satisfy the conditions requested by GUM, the authentic reference guide, we have included several statistical calculation steps and printing procedures for the uncertainty report. The program included fundamental steps such as follows; 1) editing steps for mathematical model equation of measurand, 2) steps for standard uncertainty of assigned probability density function (PDF) of each input quantity 3) steps for combined standard uncertainty with uncertainty propagation using partial derivative of each input quantity, 4) steps for extended uncertainty interval with statistical confidence level, 5) printing steps after evaluation and calculating measurement uncertainty. Including these fundamental steps, we included the calculation step of uncertainty which appears in the calibration curve using linear regression method. In the step, the standard uncertainty is calculated in the measurement incorporated by 1st order to 5th order linear regression method. In addition to describing the feature of the program, here, we presented two examples of uncertainty evaluation; one for simple comparison process of measurement, another for including 1st order linear regression process. All the results were confirmed and validated by separate procedure of calculation using Microsoft Excel.

Keywords—Measurement uncertainty, Statistical uncertainty propagation, Linear regression, Automatic report

I. INTRODUCTION

In recent years, assigning measurement uncertainty value is one of the pre-requisite for a measurement value which will be used for future important political or technical purpose[1-5]. Especially, many governments, industries and research laboratories want the quality of their measurement are assured with accreditation standard such as ISO/IEC 17025. Because this standard strictly requests well-established approach for evaluating measurement uncertainty, the 'Guide to the Expression of uncertainty in measurement (GUM)' has been widely used since it was published in 1993[1].

But many difficulties are frequently arising in the application of GUM to a real measurement case, because it includes complicated statistical steps and long tedious

preparation of report. When the GUM are applied to real measurement, there appear many simple errors in the calculation and preparing uncertainty reports. For avoiding this erroneous results, computer software has been developed and applied to the uncertainty evaluation mainly by standard research institutes and companies[6-10]. But these existing software programs have only supported for simple calculation of partial derivatives and uncertainty propagation on the positive mathematical function of model. They have not assisted any uncertainty propagation in linear regression model or negative mathematical function of measurement model[11, 12]. These programs also do not include any automatic steps of the preparation of report in connection to the evaluation process and results.

In order to overcome these difficulties, we have developed a computer program named Uncertainty-Bot. The program could be used for evaluation of uncertainty requested by GUM including uncertainty evaluation for linear regression model and reporting the result after evaluation and calculation.

For the development of the Uncertainty-Bot, C, C++ and MFC in Microsoft Visual Studio(Ver. 2015, Microsoft) were used and Microsoft Word and Microsoft PowerPoint were incorporated for word processing and graphic design. Microsoft Excel also assisted for the verification of the calculated results including partial derivatives and matrix in the software.

II. GUM GUIDE SUMMARIZED

The steps for evaluating and expressing the uncertainty as described in GUM are summarized as follows:

A. Mathematical Model of measurement

(1) Express mathematically the relationship between the measurand, Y and the input quantities X_i on which Y depends;

$$Y = f(X_1, X_2, \dots, X_i, \dots, X_n) , \quad (\text{Eq. 1})$$

where the n is number of input quantities. The function, f should contain every quantity, including all corrections and

correction factors, that can contribute any significant component of uncertainty and the result of the measurement.

(2) Determine x_i , the estimated value of input quantity X_i , either on the basis of the statistical analysis of series of observations or by other means.

(3) Calculate the result of the measurement, that is, the estimate y of the measurand Y , from the functional relationship, f using the obtained estimates x_i of the input quantities X_i . Where the equation of the estimate, y of the measurand, Y is as follows;

$$y = f(x_1, x_2, \dots, x_i, \dots, x_n) \quad (\text{Eq. 2})$$

B. Standard uncertainty and covariance

(1) Evaluate the standard uncertainty, $u(x_i)$ of each input estimate, x_i . For an input estimate obtained from the statistical analysis of series(n) of observations, the standard uncertainty($u(x_i)$) is evaluated as standard deviation(s) of the mean($\bar{x}$), described in Type A evaluation of standard uncertainty;

$$u(x_i) = \frac{s}{\sqrt{n}} = \sqrt{\frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n(n-1)}} \quad (\text{Eq. 3})$$

(2) For an input estimate obtained by other means, the standard uncertainty, $u(x_i)$ is evaluated depending on the PDF(probability density function) of the uncertainty as described in Type B evaluation of standard uncertainty;

$$u(x_i) = \frac{s}{\sqrt{3}}; \text{ for rectangular PDF.} \quad (\text{Eq. 4})$$

$$u(x_i) = \frac{s}{\sqrt{6}}; \text{ for triangular PDF.} \quad (\text{Eq. 5})$$

$$u(x_i) = \frac{s}{3}; \text{ for Gaussian PDF.} \quad (\text{Eq. 6})$$

$$u(x_i) = \frac{s}{\sqrt{2}}; \text{ for U - Shape PDF.} \quad (\text{Eq. 7})$$

(3) Evaluate the covariance and correlation coefficient associated with any input estimates that are correlated.

C. Combined standard uncertainty

(1) Determine the combined standard uncertainty, $u_c(y)$ of the measurement result, y as standard deviation of the value from the standard uncertainties associated with the input estimates, as described by uncertainty propagation step;

$$u_c^2(y) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \quad (\text{Eq. 8})$$

(2) If the measurement determines simultaneously more than one output quantity, obtain their correlation coefficient(r_{ij}) values and use uncertainty propagation step as follows;

$$\begin{aligned} u_c^2(y) &= \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \\ &+ 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \left(\frac{\partial f}{\partial x_i} \right) \left(\frac{\partial f}{\partial x_j} \right) u(\partial x_i) u(\partial x_j) r_{ij} \end{aligned} \quad (\text{Eq. 9})$$

D. Expanded uncertainty

(1) Calculate an expanded uncertainty, U , whose purpose is to provide an statistical confidence interval, $y - U$ to $y + U$ that may be encompassed a expected fraction of the distribution of uncertainty that could reasonably be attributed to the measurand, Y as follows;

$$U = k \cdot u_c(y), \quad (\text{Eq. 10})$$

(2) Select coverage factor, k on the basis of the level of confidence and degrees of freedom required for the statistical interval from estimated PDF of the measurand.

E. Reporting uncertainty

(1) Explain the estimator, y , of the measurement together with its expanded uncertainty, U and selected confidence level.

(2) Report the appropriate details of uncertainty evaluation.

III. FEATURE OF UNCERTAINTY-BOT

Uncertainty-Bot developed is a computer program used for measurement uncertainty which is complied with criteria of GUM. It works at Microsoft Window 7 and 10 and the first log and main windows are shown at Figure 1.

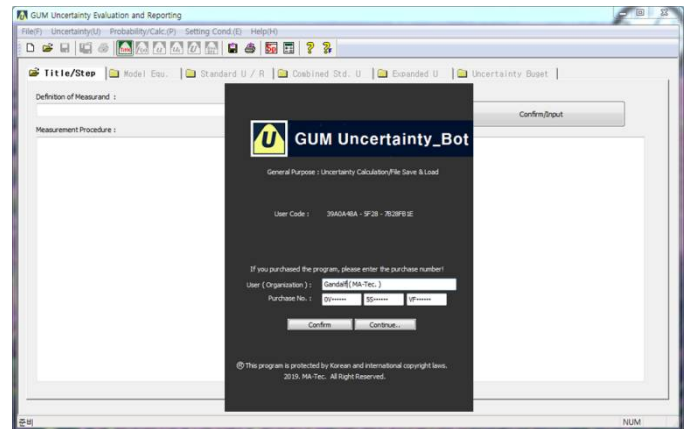


Figure 1. First log and main windows of Uncertainty-Bot

For evaluating uncertainty, six windows with tabs are provided as follows;

- (1) Title tab for entering the title and description of measurement procedure as shown in Figure 1,
- (2) Equation tab for inputting the mathematical equation of measurand(Eq. 2); an example of model equations is presented in Figure 2.
- (3) Standard uncertainty tab for calculating standard uncertainty for assigned PDF(Eq. 3 -Eq. 7) and correlation coefficients; an example of standard uncertainty tab is presented also in Figure 2, and various PDFs provided are illustrated with graphs shown in Figure 3,

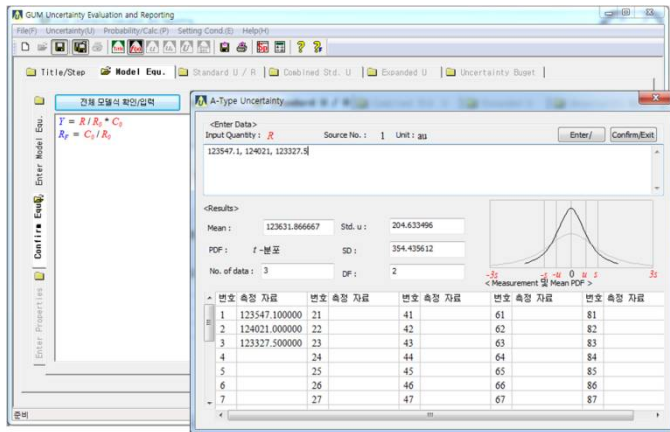


Figure 2. Example of windows provided by Uncertainty-Bot

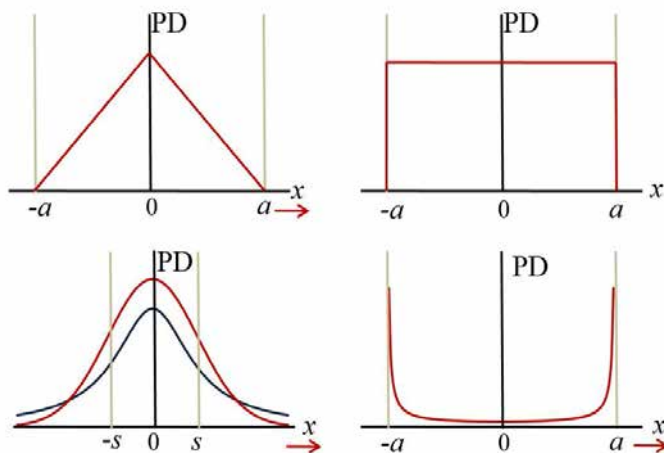


Figure 3. Examples of various assigned PDFs

- (4) Combined standard uncertainty tab for calculating partial derivatives and combined standard uncertainty through uncertainty propagation formulae(Eq. 8 - Eq. 9),
- (5) Extended uncertainty tab for providing coverage factor depending on the confidence level and effective degrees of freedom, and calculating extended uncertainty value(Eq. 10),

- (6) Uncertainty-budget tab for comparing relative contribution ratio values between input uncertainty components.

After Uncertainty-budget, Uncertainty-Bot can provide a printed report with all the results of evaluation and one of the report style is resented as shown in Figure 4.

Table. Uncertainty Budget

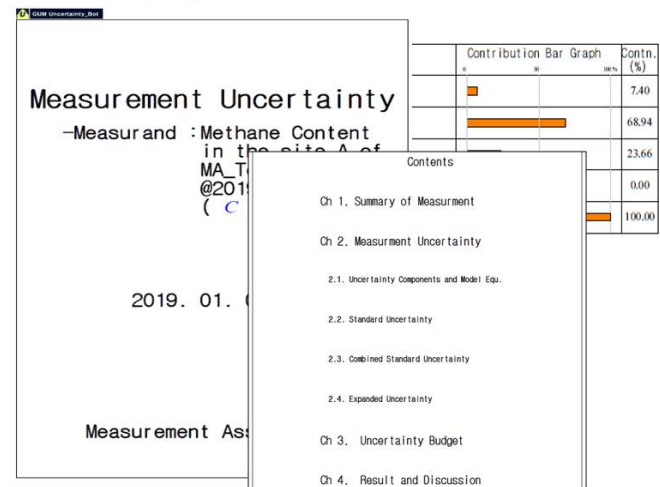


Figure 4. Example of the report provided by Uncertainty-Bot

In addition to these fundamental steps, Uncertainty-Bot also provides steps in which calibration curve are calculated by least square method and combined standard uncertainty of the measurement result obtained with the calibration curve. The process includes calibration curve from 1st order to 5th order equation. The equation of combined standard uncertainty($u(x)$) in the measurement with 1st order linear regression is the one shown in Eq. 11, where calibration line(y) and standard deviation(s) are those written in Eq. 12 and in Eq. 13[12]. In the equations, n is number of regression data, p is number of repetition data of measurement, b_1 is slope and b_0 is intercept of the 1st order calibration line, and (y_i, x_i) are i th regression data pair.

$$u(x) = \frac{s}{b_1} \sqrt{\frac{1}{p} + \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (\text{Eq. 11})$$

$$y = b_1 x + b_0 \quad (\text{Eq. 12})$$

$$s = \sqrt{\frac{\sum \{y_i - (b_1 x_i + b_0)\}^2}{n - 2}} \quad (\text{Eq. 13})$$

The equation of combined standard uncertainty($u(x)$) in the measurement with the calibration curve of high order linear regression is the one written in Eq. 14, where the calibration curve, component of inverse matrix(M_{ij}) and standard deviation(s) are those written in Eq. 15, Eq. 16 and Eq. 17[12]. And y' is slope of tangent line, m is order of calibration curve and, $b_m, \dots, b_1$ and b_0 are coefficients of the equation.

IV. EXAMPLE 1

In order to check Uncertainty-Bot working properly, we evaluated the uncertainty of a measurand; mole fraction of methane in a factory ambient air and compare them with the results calculated only with Microsoft Excel, for which measurement data are such as those summarized at Table 1.

TABLE 1. MEASUREMENT CONDITION AND DATA FOR EXAMPLE 1

	Item	Measurement Details
1	Measurand	Mole fraction of methane in ambient air
2	Method	Non-dispersive IR methane analyser
3	Procedure	1) One-Point calibration with reference gas (Certified mole fraction of CH ₄ , 451.5 μmol/mol) 2) Determine response factor of the analyser 3) Determine mole fraction of CH ₄ 1) Standard uncertainty of reference gas (4.5 μmol/mol); 2) Sequential response values of reference gas (417.8, 418.4, 416.5 and Mean, 417.6) 3) Response factor from calibration process, 451.5/417.6 = 1.01813
4	Results	1) Measurement data; Sequential response values of ambient air (127.8, 130.4, 128.5 and Mean, 128.9) 2) Estimated value of measurand (1.01813 x 128.9 = 139.37 (μmol/mol))

As a first step using Uncertainty-Bot, we input two equations as shown in Eq. 18 and Eq. 19.

C = R_f · R_{smpl} (Eq. 18)

R_f = C_{ref} / R_{ref} (Eq. 19)

where C is measurand (mole fraction of ambient air), R_f is response factor of the analyser, C_{ref} is certified mole fraction of the reference gas, R_{ref} is response of reference gas and R_{smpl} is response of ambient air.

After mathematical modelling, each standard uncertainty and degrees of freedom were calculated using Uncertainty-Bot using the equation from Eq. 3 – Eq. 7, and the results were summarized with estimated value of input quantity at Table. 2.

TABLE 2. SUMMARY OF STANDARD UNCERTAINTY IN THE MEASUREMENT OF METHANE MOLE FRACTION IN AIR

	Estimated value	Standard uncertainty	Degrees of freedom
1	C _{ref} = 451.5 μmol/mol	u(C _{ref}) = 4.50 μmol/mol	∞
2	R _{ref} = 417.6	u(R _{ref}) = 0.561	2
3	R _{ref} = 128.9	u(C _{ref}) = 0.777	2

u(x) = (s / y') * sqrt(1/p + sum_{i=1}^m sum_{j=1}^m M_{ij} x^{(i+j)}) (Eq. 14)

y = b_mx^m + ... + b₁x + b₀ (Eq. 15)

[M_{ij}] = [sum_{i=1}^n x_i^n, sum_{i=1}^n x_i^{n+1}, ..., sum_{i=1}^n x_i^{2n}]^{-1} (Eq. 16)

s = sqrt(sum_{i=1}^n {y_i - (b_mx_i^m + ... + b₁x_i + b₀)}^2 / (n - m - 1)) (Eq. 17)

Uncertainty-Bot provides automatic calculation of the measurement including regression process and it also provides the calibration graphs depending on the type of uncertainty. As an example, combined standard uncertainty of a chemical measurement is presented in Figure 5, where the gray line is calibration curve of first order regression and red line is associated combined standard uncertainty at each determined value in the range of calibration. The orange line indicate component value of uncertainty originating from randomness of regression, whereas violet line shows value originating from uncertainty of references.

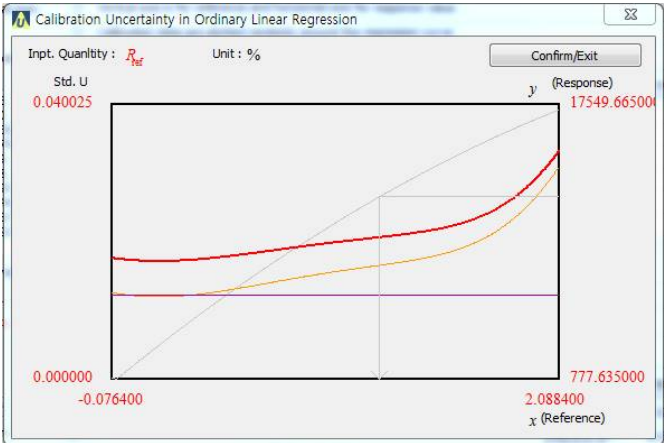


Figure 5. Examples of combined uncertainty provided by Uncertainty-Bot

With the data on the standard uncertainty values obtained, effective degrees of freedom[1] and combined standard uncertainty and expanded uncertainty were calculated using Uncertainty-Bot using the Eq. 8 and Eq. 10, and the results were summarized with estimated value of output quantity at Table. 3. These results were compared with calculated values obtained by Microsoft Excel and confirmed the reliability of Uncertainty-Bot.

TABLE 3. COMBINED STANDARD UNCERTAINTY AND EXPANDED UNCERTAINTY IN THE MEASUREMENT OF METHANE

Estimated value	Uncertainty	Remarks
Mole fraction of CH ₄ in ambient air, C = 139.4 μmol/mol	Combined standard uncertainty, $u(C) = 1.6 \mu\text{mol/mol}$	Degrees of freedom, $\nu_{\text{eff}} = 28$
	Expanded uncertainty, $U = 3.4 \mu\text{mol/mol}$	Level of confidence, 95 %, $k=2.1$

V. EXAMPLE 2

In order to check Uncertainty-Bot working properly with linear regression, the data were quoted from the GUM guide [3]: Annex H, Example H.3: Calibration of a thermometer and all the calibration data with slight arrangement were summarized at Table 4.

TABLE 4. TEMPERATURE CALIBRATION DATA

Reference	Certified Reference value(°C)	Response value (°C)	Standard Uncertainty (°C)
TStd1	21.350	21.521	0.0015
TStd2	21.843	22.012	0.0015
TStd3	22.346	22.512	0.0015
TStd4	22.844	23.003	0.0015
TStd5	23.343	23.507	0.0015
TStd6	23.834	23.999	0.0015
TStd7	24.357	24.513	0.0015
TStd8	24.845	25.002	0.0015
TStd9	25.344	25.503	0.0015
TStd10	25.849	26.010	0.0015
TStd11	26.351	26.511	0.0015

This example illustrates the evaluation of uncertainty for the calibration and predicted correction of temperature by least square method. To compare the results, the slope and intercept of calibration curve were derived by Uncertainty-Bot with reference and response temperature values from Table. 4 as shown in Figure 6.

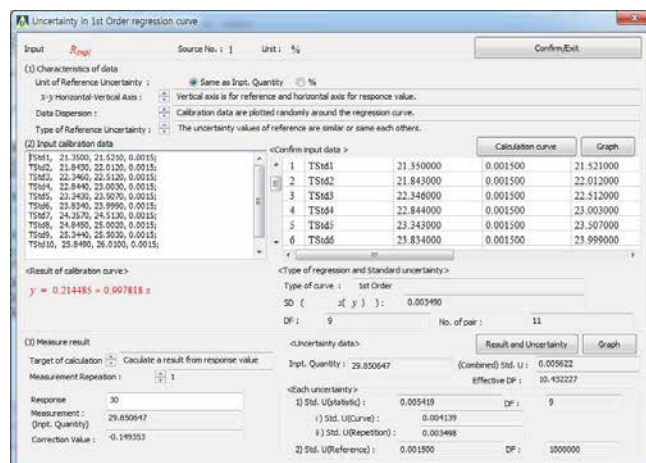


Figure 6. Examples of combined uncertainty

After calculating the calibration curve shown in Eq. 20 where y axis is response and x axis is reference, corrected temperature at response temperature, 30 °C was calculated and combined uncertainty was obtained using the program. The value of correction and associated combined standard uncertainty were as shown in Eq. 21 and Eq. 22.

$$y = 0.2145 + 0.9978 x \quad (\text{Eq. 20})$$

$$\text{Correction value(at } 30^\circ\text{C)} = -0.1494 \quad (\text{Eq. 21})$$

$$u_c(t) = 0.004139^\circ\text{C} \quad (\text{Eq. 22})$$

Uncertainty-Bot could provide a graph of combined standard uncertainty at various temperature value so that the graph was presented in Figure 7, where the gray line is calibration curve of first order regression and red line is associated combined standard uncertainty at each determined value in the range of calibration. The orange line indicates an uncertainty component originating from randomness of regression, whereas violet line originating from uncertainty of references. All these results were compared with values described at GUM and confirmed the reliability of Uncertainty-Bot.

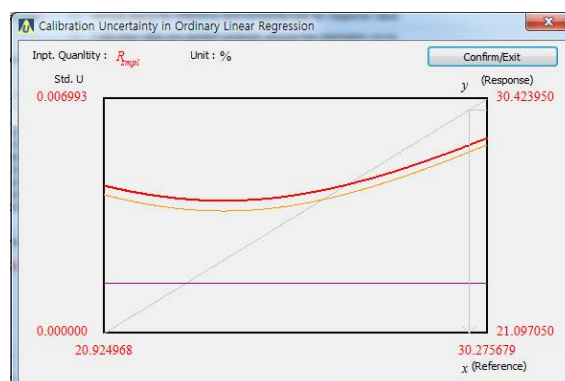


Figure 7. Example of combined uncertainty

VI. CONCLUSIONS

For the evaluation of measurement uncertainty and preparation of a report connecting to the results, Uncertainty-Bot has been developed. In this study, we confirmed the reliability and usability of the program. We hope this program would be used in many science fields and industrial areas for the quality assurance of measurement.

In recent years, Monte-Carlo simulation is widely used for the uncertainty calculation when the left and right side of PDF is not mirror image[11, 13]. Therefore, we plan several studies including the Monte-Carlo simulation and up-grading the user interfacing work of Uncertainty-Bot.

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